CS 267 Applications of Parallel Computers

Lecture 10:

Sources of Parallelism and Locality (Part 2)

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based on previous lecture notes by Jim Demmel and Dave Culler

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Recap of last lecture

- Simulation models
- A model problem: sharks and fish
- Discrete event systems
- Particle systems
- Lumped systems - ordinary differential equations (ODEs)

Outline

- Continuation of (ODEs)
- Partial Differential Equations (PDEs)

Ordinary Differential Equations
ODEs

Solving ODEs

- **Explicit methods to compute solution(t)**
  - **Example: Euler's method.**
  - **Simple algorithm: sparse matrix vector multiply.**
  - **May need to take very small time steps, especially if system is stiff (i.e. can change rapidly).**
- **Implicit methods to compute solution(t)**
  - **Example: Backward Euler's Method.**
  - **Larger timesteps, especially for stiff problems.**
  - **More difficult algorithm: solve a sparse linear system.**
- **Computing modes of vibration**
  - **Finding eigenvalues and eigenvectors.**
  - **Example: do resonant modes of building match earthquakes?**
- **All these reduce to sparse matrix problems**
  - **Explicit: sparse matrix-vector multiplication.**
  - **Implicit: solve a sparse linear system**
    - **direct solvers (Gaussian elimination).**
    - **iterative solvers (use sparse matrix-vector multiplication).**
  - **Eigenvalue/vector algorithms may also be explicit or implicit.**

Solving ODEs - Details

- Assume ODE is x'(t) = f(x) = A*x, where A is a sparse matrix
  - Try to compute x(i*dt) = x[i] at i=0,1,2,…
  - Approximate x'(i*dt) by (x[i+1] - x[i])/dt
- Euler's method:
  - Approximate x'(t)=A*x by (x[i+1] - x[i])/dt = A*x[i] and solve for x[i+1].
  - x[i+1] = (I+dt*A)*x[i], i.e. sparse matrix-vector multiplication.
- Backward Euler's method:
  - Approximate x'(t)=A*x by (x[i+1] - x[i])/dt = A*x[i+1] and solve for x[i+1].
  - (I - dt*A)*x[i+1] = x[i], i.e. we need to solve a sparse linear system of equations.
- Modes of vibration
  - Seek solution of x''(t) = A*x of form x(t) = sin(f*t)*x0, where x0 is a constant vector.
  - Plug in to get -f *x0 = A*x0, so that -f is an eigenvalue and x0 is an eigenvector of A.
  - Solution schemes reduce either to sparse-matrix multiplication, or solving sparse linear systems.

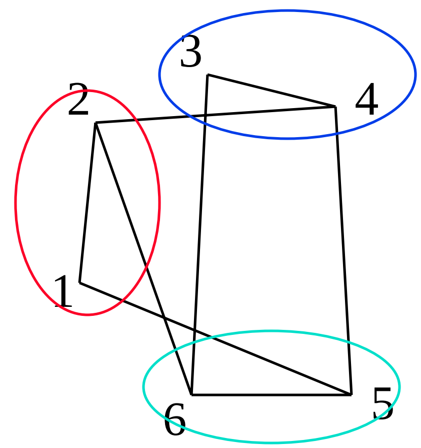
Parallelism in Sparse Matrix-vector multiplication

- y = A*x, where A is sparse and n x n
- Questions
  - which processors store
    - y[i], x[i], and A[i,j]
  - which processors compute
    - y[i] = sum (from 1 to n) A[i,j] * x[j]
      = (row i of A) * x … a sparse dot product
- Partitioning
  - Partition index set {1,…,n} = N1 u N2 u … u Np.
  - For all i in Nk, Processor k stores y[i], x[i], and row i of A
  - For all i in Nk, Processor k computes y[i] = (row i of A) * x
    - "owner computes" rule: Processor k compute the y[i]s it owns.
- Goals of partitioning
  - balance load (how is load measured?).
  - balance storage (how much does each processor store?).
  - minimize communication (how much is communicated?).

Graph Partitioning and Sparse Matrices

- **Relationship between matrix and graph**

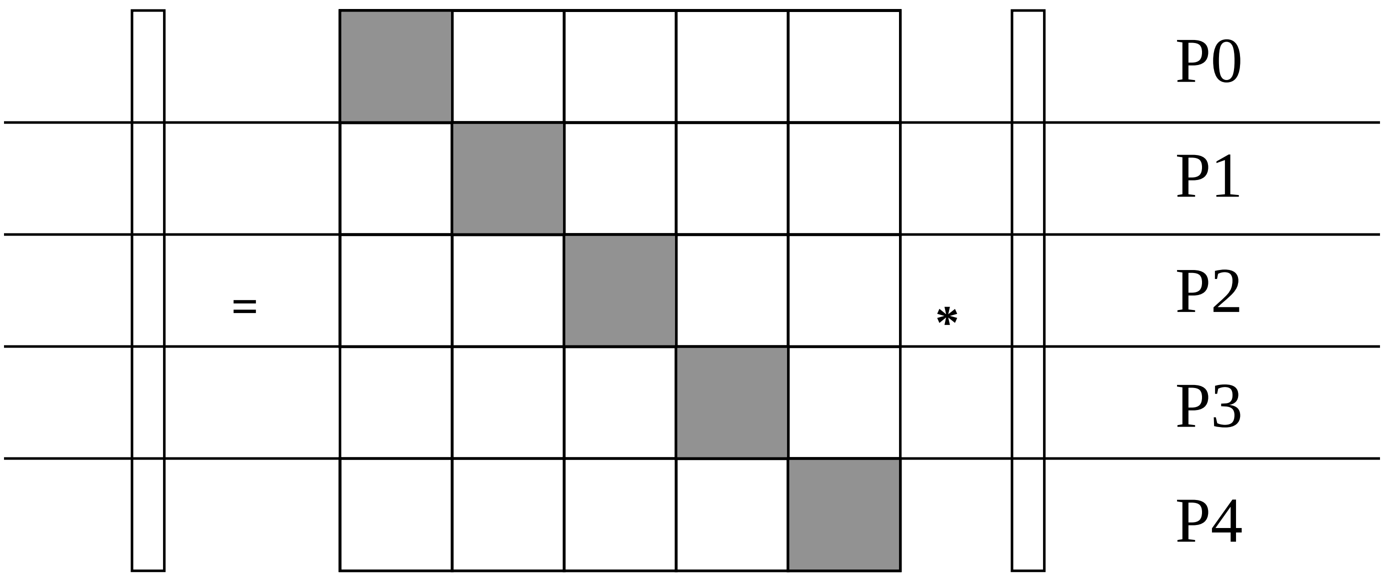
$$
\begin{array}{c|cccccc|}
 & 1 & 2 & 3 & 4 & 5 & 6 \\
\hline
1 & 1 & 1 & & & 1 & \\
2 & 1 & 1 & & 1 & & 1 \\
3 & & & 1 & 1 & & 1 \\
4 & & 1 & 1 & 1 & 1 & \\
5 & 1 & & & 1 & 1 & 1 \\
6 & & 1 & 1 & & 1 & 1 \\
\hline
\end{array}
$$



- **A "good" partition of the graph has**
  - **equal (weighted) number of nodes in each part (load and storage balance).**
  - **minimum number of edges crossing between (minimize communication).**
- **Can reorder the rows/columns of the matrix by putting all the nodes in one partition together.**

More on Matrix Reordering via Graph Partitioning

° **"Ideal" matrix structure for parallelism: (nearly) block diagonal**
  - **p (number of processors) blocks.**
  - **few non-zeros outside these blocks, since these require communication.**



What about implicit methods and eigenproblems?

- **Direct methods (Gaussian elimination)**
  - **Called LU Decomposition, because we factor A = L*U.**
  - **Future lectures will consider both dense and sparse cases.**
  - **More complicated than sparse-matrix vector multiplication.**
- **Iterative solvers**
  - **Will discuss several of these in future.**
    - **Jacobi, Successive overrelaxiation (SOR) , Conjugate Gradients (CG), Multigrid,...**
  - **Most have sparse-matrix-vector multiplication in kernel.**
- **Eigenproblems**
  - **Future lectures will discuss dense and sparse cases.**
  - **Also depend on sparse-matrix-vector multiplication, direct methods.**
- **Graph partitioning**
  - **Algorithms will be discussed in future lectures.**

Partial Differential Equations

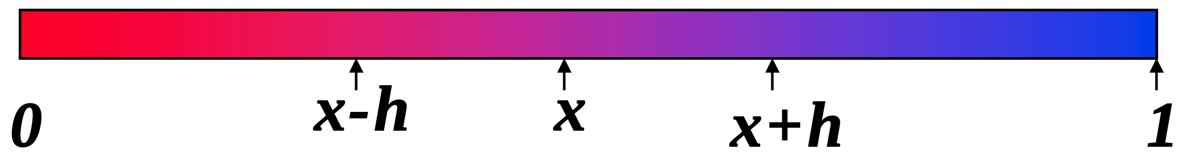
PDEs

Continuous Variables, Continuous Parameters

Examples of such systems include

- **Heat flow:** Temperature(position, time)
- **Diffusion:** Concentration(position, time)
- **Electrostatic or Gravitational Potential:**
  Potential(position)
- **Fluid flow:** Velocity,Pressure,Density(position,time)
- **Quantum mechanics:** Wave-function(position,time)
- **Elasticity:** Stress,Strain(position,time)

Example: Deriving the Heat Equation



Consider a simple problem

- A bar of uniform material, insulated except at ends
- Let $u(x,t)$ be the temperature at position x at time t
- Heat travels from x-h to $x+h$ at rate proportional to:

$$\frac{d\ u(x,t)}{dt} = C * \frac{(u(x-h,t)-u(x,t))/h - (u(x,t)- u(x+h,t))/h}{h}$$

- As $h \rightarrow 0$, we get the heat equation:

$$\frac{d\ u(x,t)}{dt} = C * \frac{d^2\ u(x,t)}{dx^2}$$

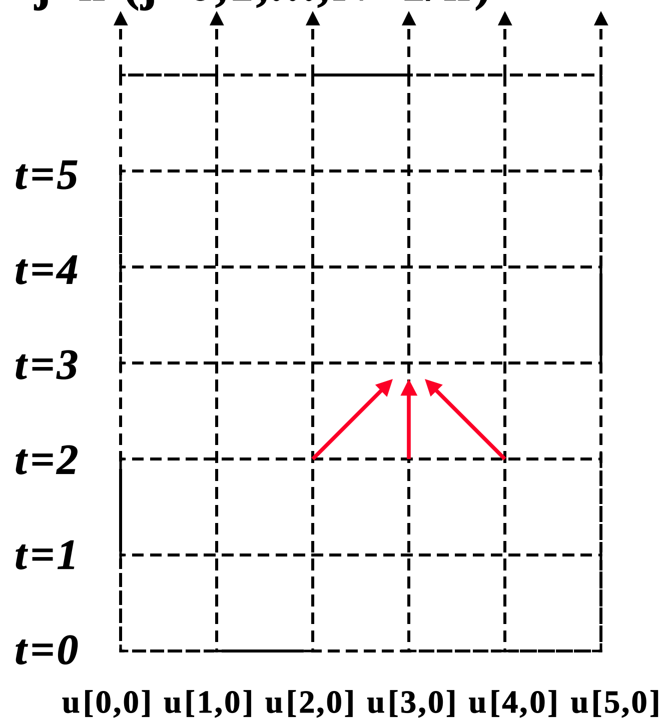
Explicit Solution of the Heat Equation

- For simplicity, assume $C=1$
- Discretize both time and position
- Use finite differences with u[j,i] as the heat at
  - time t= i*dt (i = 0,1,2,…) and position x = j*h (j=0,1,…,N=1/h)
  - initial conditions on u[j,0]
  - boundary conditions on u[0,i] and u[N,i]
- At each timestep i = 0,1,2,...

For j=0 to N

u[j,i+1]= z*u[j-1,i]+ (1-2*z)*u[j,i]+ z*u[j+1,i]

where z = dt/h^2

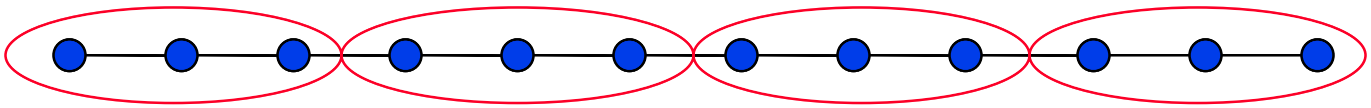


- This corresponds to
  - matrix vector multiply (what is matrix?)
  - nearest neighbors on grid

Parallelism in Explicit Method for PDEs

° **Partitioning the space (x) into p largest chunks**

- good load balance (assuming large number of points relative to p)
- minimized communication (only p chunks)



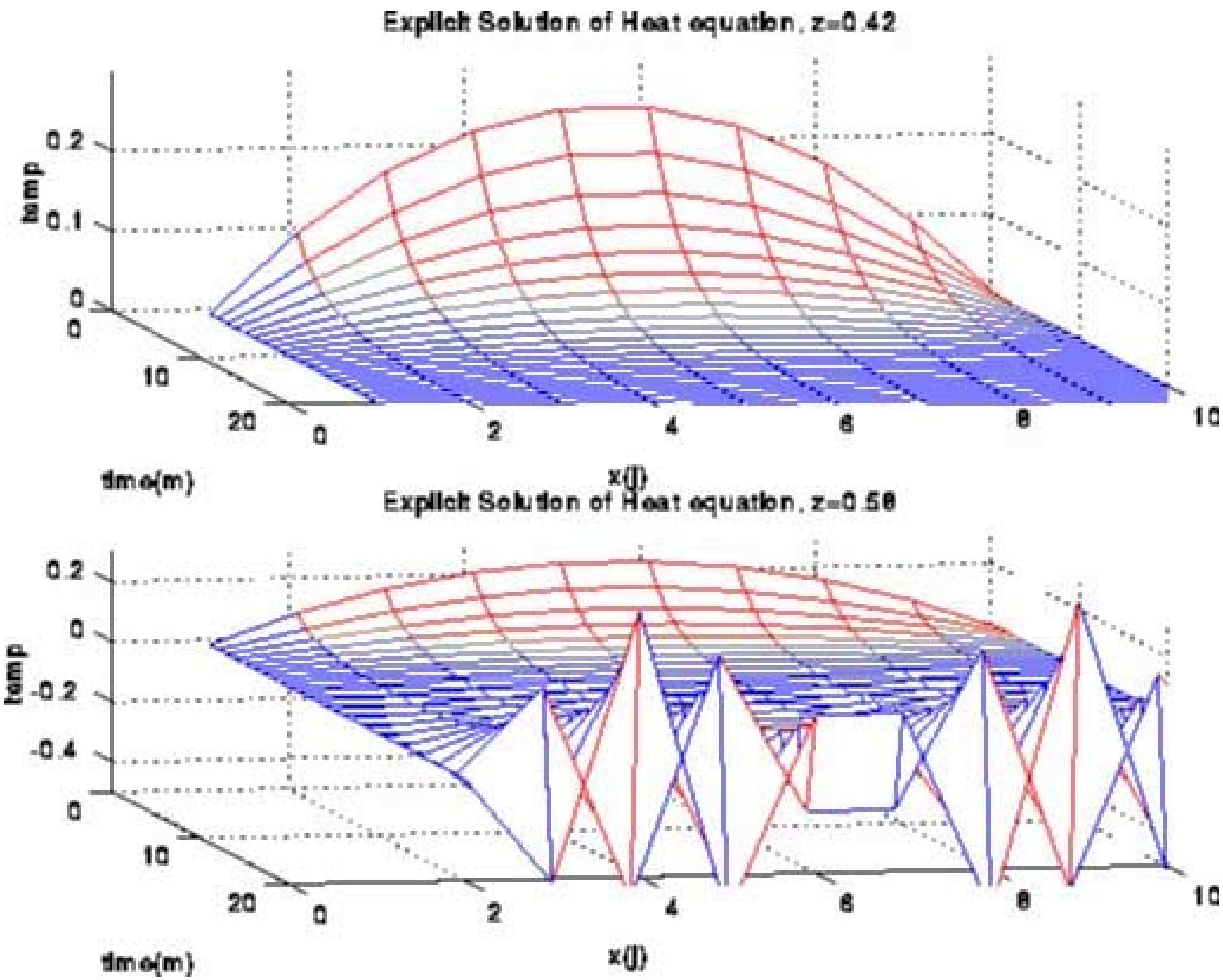
° **Generalizes to**

- multiple dimensions.
- arbitrary graphs (= sparse matrices).

° **Problem with explicit approach**

- numerical instability.
- solution blows up eventually if $z = dt/h^2 > .5$
- need to make the time steps very small when h is small: $dt < .5*h^2$

Instability in solving the heat equation explicitly



Implicit Solution

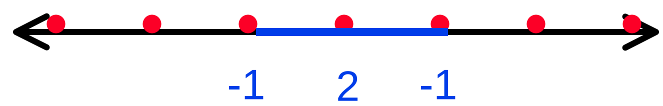
- As with many (stiff) ODEs, we need to use an implicit method.
- This turns into solving the following equation:

  (I + (z/2)*T) * u[:,i+1]= (I - (z/2)*T) *u[:,i]

- Here I is the identity matrix and T is:

$$
T = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}
$$

Graph and "stencil"



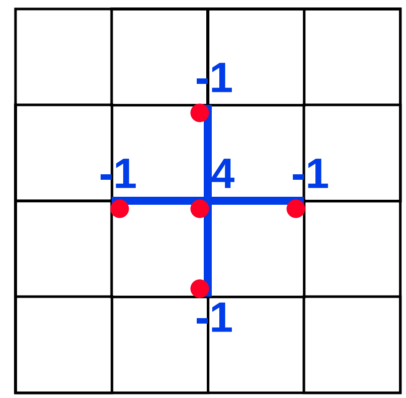
- I.e., essentially solving Poisson's equation in 1D

2D Implicit Method

- **Similar to the 1D case, but the matrix T is now**

$$T = \left(\begin{array}{ccc|ccc|ccc}
4 & -1 & & -1 & & & & & \\
-1 & 4 & -1 & & -1 & & & & \\
& -1 & 4 & & & -1 & & & \\
\hline
-1 & & & 4 & -1 & & -1 & & \\
& -1 & & -1 & 4 & -1 & & -1 & \\
& & -1 & & -1 & 4 & & & -1 \\
\hline
& & & -1 & & & 4 & -1 & \\
& & & & -1 & & -1 & 4 & -1 \\
& & & & & -1 & & -1 & 4
\end{array}\right)$$

Graph and "stencil"



- **Multiplying by this matrix (as in the explicit case) is simply nearest neighbor computation on 2D grid.**
- **To solve this system, there are several techniques.**

Algorithms for 2D Poisson Equation with N unknowns

Algorithm	Serial	PRAM	Memory	#Procs
° Dense LU	N^3	N	N^2	N^2
° Band LU	N^2	N	$N^{3/2}$	N
° Jacobi	N^2	N	N	N
° Explicit Inv.	N^2	log N	N^2	N^2
° Conj.Grad.	$N^{3/2}$	$N^{1/2} *\log N$	N	N
° RB SOR	$N^{3/2}$	$N^{1/2}$	N	N
° Sparse LU	$N^{3/2}$	$N^{1/2}$	N*log N	N
° FFT	N*log N	log N	N	N
° Multigrid	N	$\log^2 N$	N	N
° Lower bound	N	log N	N	

PRAM is an idealized parallel model with zero cost communication

(see next slide for explanation)

Short explanations of algorithms on previous slide

- **Sorted in two orders (roughly):**
  - **from slowest to fastest on sequential machines.**
  - **from most general (works on any matrix) to most specialized (works on matrices “like” T).**
- **Dense LU: Gaussian elimination; works on any N-by-N matrix.**
- **Band LU: Exploits the fact that T is nonzero only on sqrt(N) diagonals nearest main diagonal.**
- **Jacobi: Essentially does matrix-vector multiply by T in inner loop of iterative algorithm.**
- **Explicit Inverse: Assume we want to solve many systems with T, so we can precompute and store inv(T) “for free”, and just multiply by it (but still expensive).**
- **Conjugate Gradient: Uses matrix-vector multiplication, like Jacobi, but exploits mathematical properties of T that Jacobi does not.**
- **Red-Black SOR (successive over-relaxation): Variation of Jacobi that exploits yet different mathematical properties of T. Used in multigrid schemes.**
- **LU: Gaussian elimination exploiting particular zero structure of T.**
- **FFT (fast Fourier transform): Works only on matrices *very* like T.**
- **Multigrid: Also works on matrices like T, that come from elliptic PDEs.**
- **Lower Bound: Serial (time to print answer); parallel (time to combine N inputs).**
- **Details in class notes and www.cs.berkeley.edu/~demmel/ma221.**

Relation of Poisson's Equation to Gravity, Electrostatics

° Force on particle at (x,y,z) due to particle at 0 is

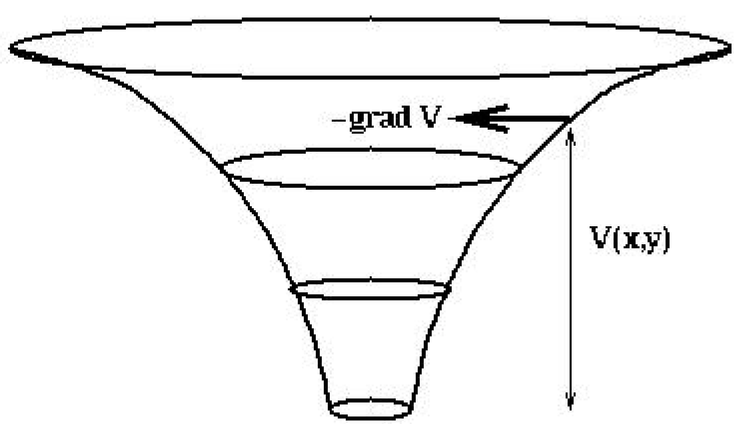
$-(x,y,z)/r^3$, where $r = \mathrm{sqrt}(x^2+y^2+z^2)$

° Force is also gradient of potential $V = -1/r$

$= -(d/dx\ V,\ d/dy\ V,\ d/dz\ V) = -\mathrm{grad}\ V$

° V satisfies Poisson's equation (try it!)

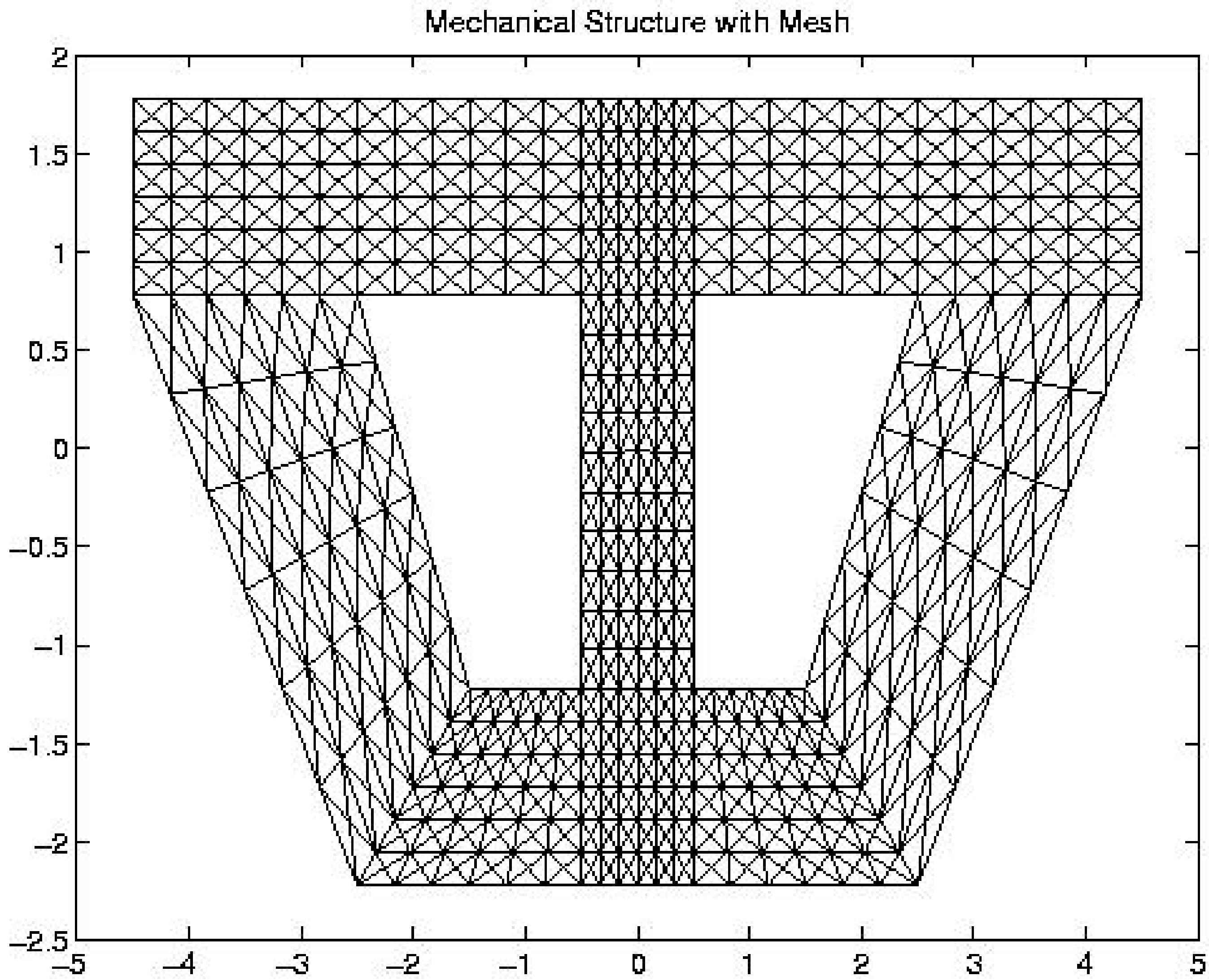
Relationship of Potential V and Force –grad V in 2D



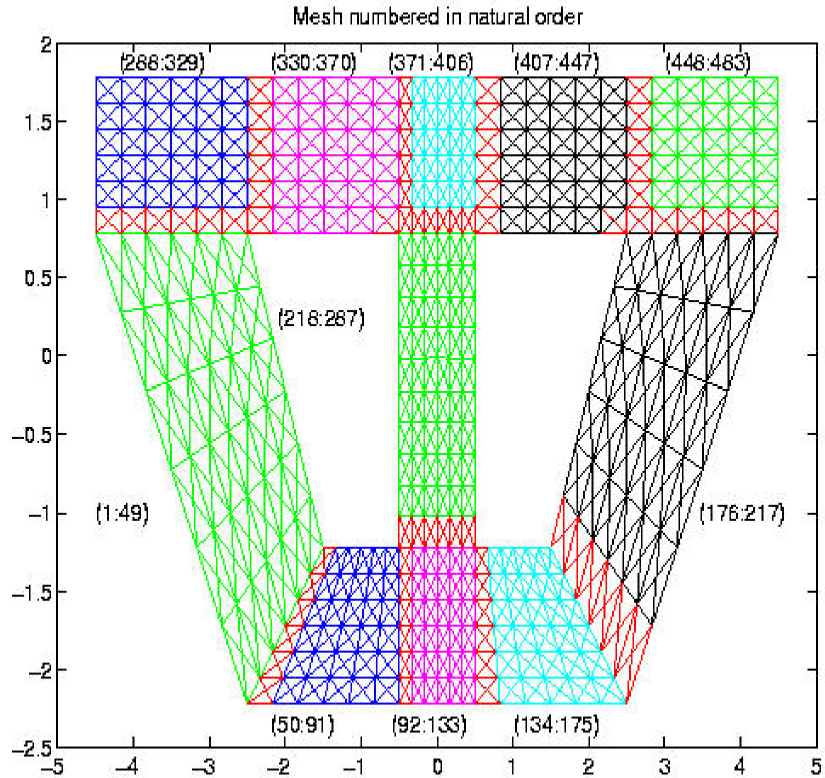
Comments on practical meshes

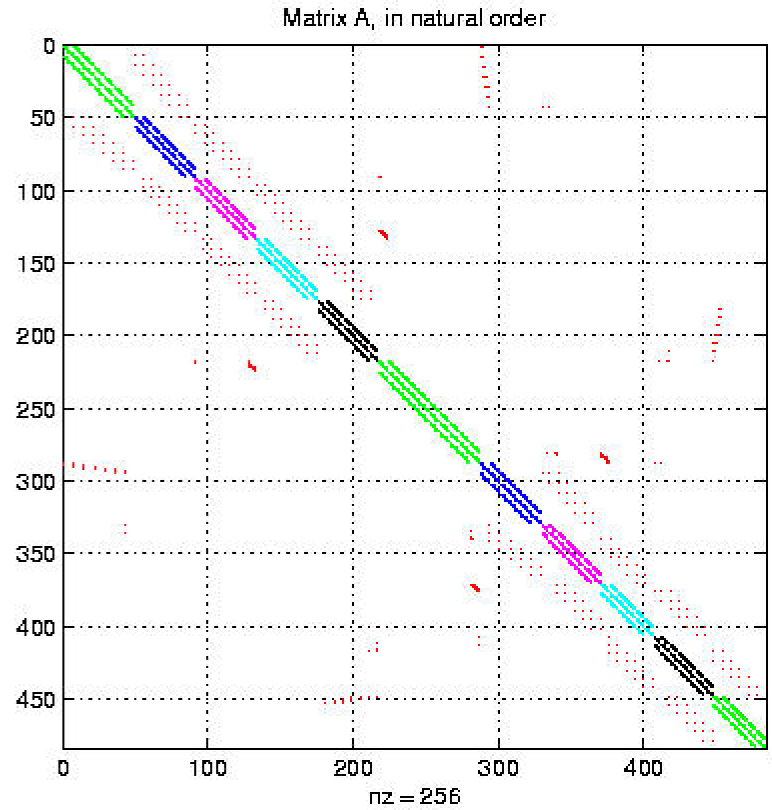
- **Regular 1D, 2D, 3D meshes**
  - **Important as building blocks for more complicated meshes.**
- **Practical meshes are often irregular**
  - **Composite meshes, consisting of multiple “bent” regular meshes joined at edges.**
  - **Unstructured meshes, with arbitrary mesh points and connectivity.**
  - **Adaptive meshes, which change resolution during solution process to put computational effort where needed.**

Composite mesh from a mechanical structure

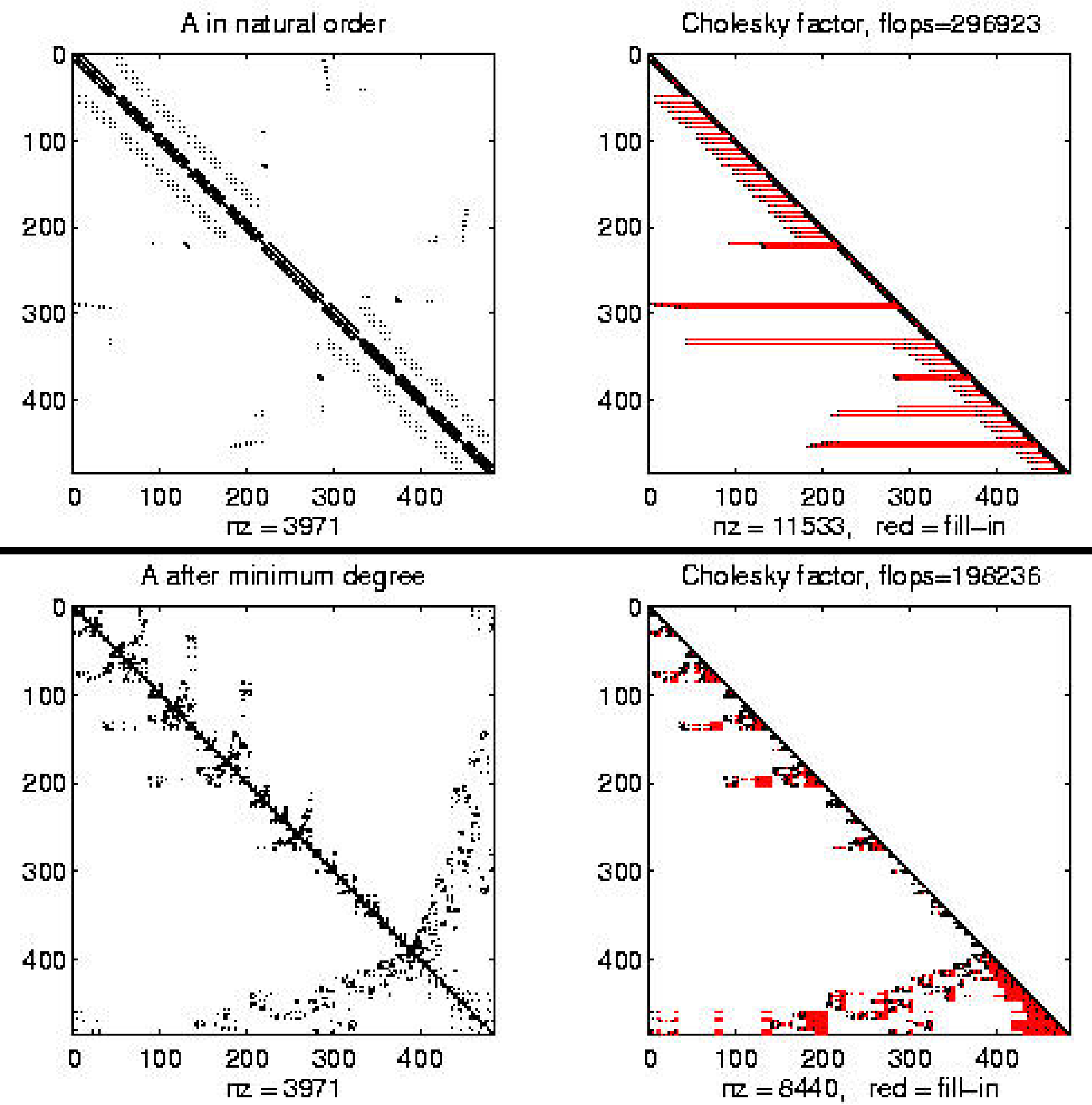


Converting the mesh to a matrix

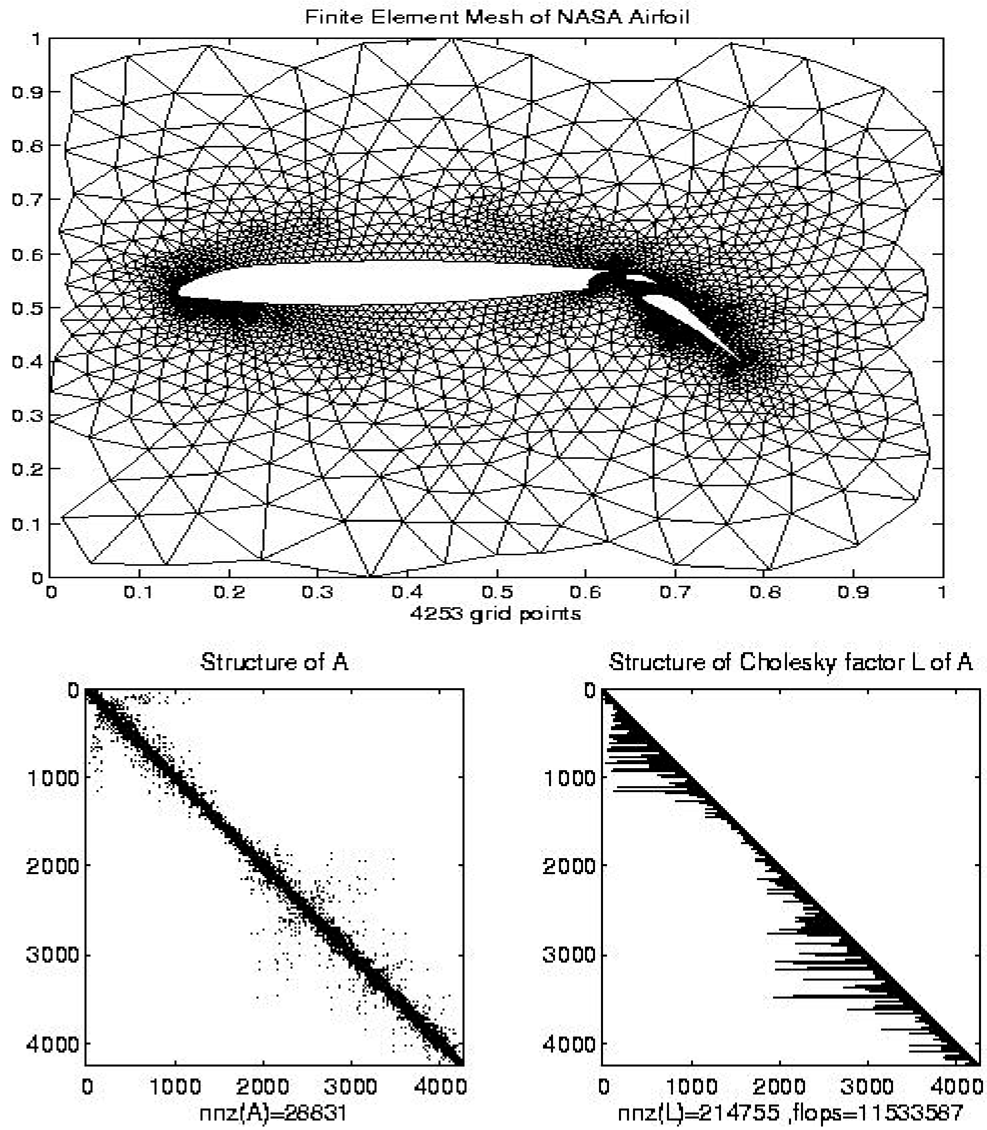




Effects of Ordering Rows and Columns on Gaussian Elimination



Irregular mesh: NASA Airfoil in 2D (direct solution)



Irregular mesh: Tapered Tube (multigrid)

Example of Prometheus meshes

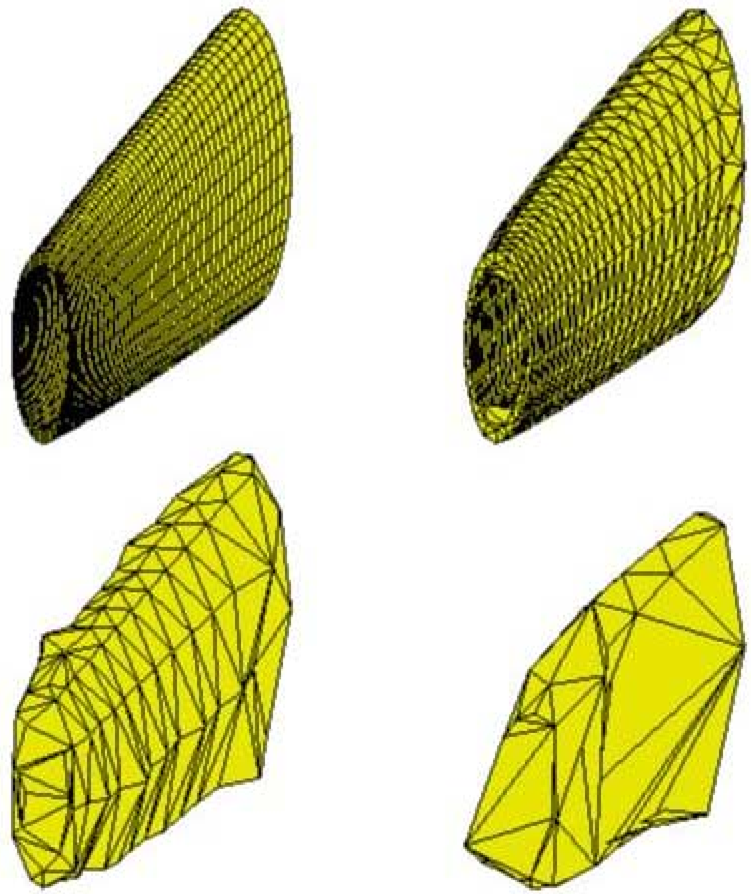
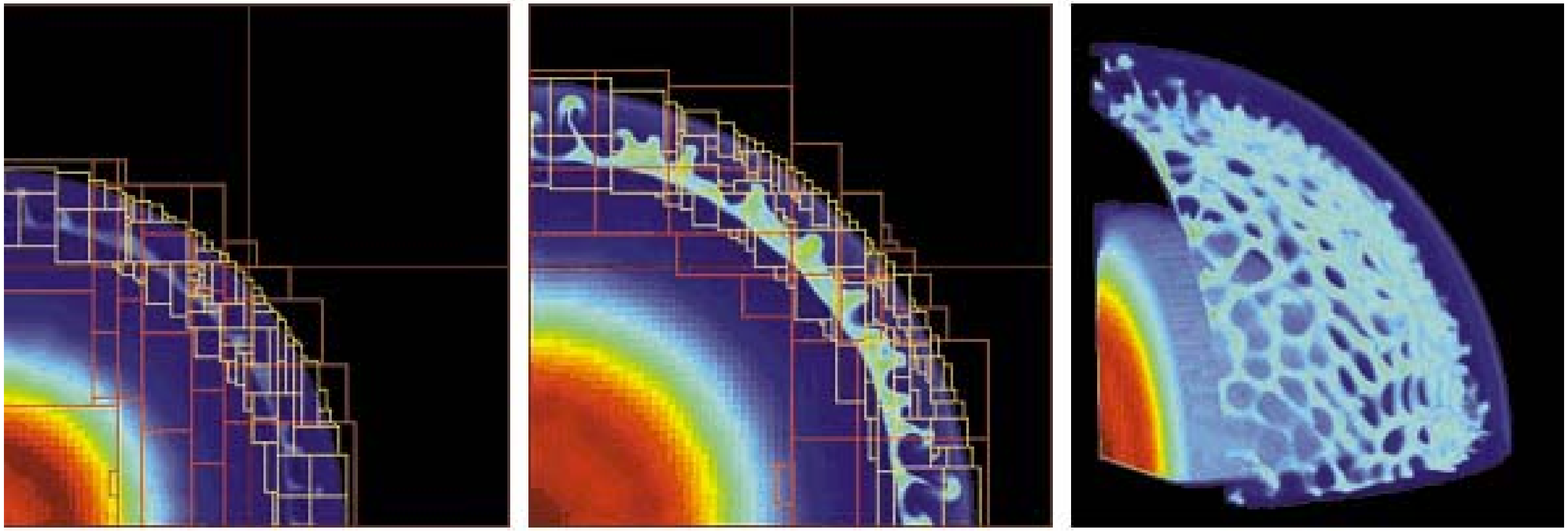


Figure 6: Sample input grid and coarse grids

Adaptive Mesh Refinement (AMR)



- Adaptive mesh around an explosion.
- John Bell and Phil Colella at LBL/NERSC.
- Goal of Titanium is to make these algorithms easier to implement in parallel.

Challenges of irregular meshes (and a few solutions)

- **How to generate them in the first place:**
  - **Triangle, a 2D mesh partitioner by Jonathan Shewchuk.**
- **How to partition them:**
  - **ParMetis, a parallel graph partitioner.**
- **How to design iterative solvers:**
  - **PETSc, a Portable Extensible Toolkit for Scientific Computing.**
  - **Prometheus, a multigrid solver for finite element problems on irregular meshes.**
  - **Titanium, a language to implement Adaptive Mesh Refinement.**
- **How to design direct solvers:**
  - **SuperLU, parallel sparse Gaussian elimination.**
- **These are challenges to do sequentially, the more so in parallel.**